Butane, 2-methyl-3-(methylthio)-

Other names: 3,4-Dimethyl-2-thiapentane
Methyl (1,2-dimethylpropyl) sulfide
Inchi: InChI=1S/C6H14S/c1-5(2)6(3)7-4/h5-6H,1-4H3
InchiKey: AUNQXXJGFDKEMS-UHFFFAOYSA-N
Formula: C6H14S
SMILES: CSC(C)C(C)C
Mol. weight [g/mol]: 118.24
CAS: 53897-51-1

Physical Properties

Property code	Value	Unit	Source
gf	27.88	kJ/mol	Joback Method
hf	-135.86	kJ/mol	Joback Method
hfus	8.38	kJ/mol	Joback Method
hvap	34.99	kJ/mol	Joback Method
log10ws	-2.09		Crippen Method
logp	2.394		Crippen Method
mcvol	111.750	ml/mol	McGowan Method
pc	3224.64	kPa	Joback Method
rinpol	862.00		NIST Webbook
rinpol	862.00		NIST Webbook
rinpol	862.00		NIST Webbook
rinpol	862.00		NIST Webbook
tb	404.58	K	Joback Method
tc	602.65	K	Joback Method
tf	161.78	K	Joback Method
vc	0.413	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	206.45	J/mol×K	404.58	Joback Method
cpg	218.68	J/mol×K	437.59	Joback Method
cpg	230.42	J/mol×K	470.60	Joback Method

cpg	241.66	J/mol×K	503.61	Joback Method
cpg	252.43	J/mol×K	536.62	Joback Method
cpg	262.72	J/mol×K	569.63	Joback Method
cpg	272.54	J/mol×K	602.65	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.44961e+01
Coeff. B	-3.47042e+03
Coeff. C	-5.26700e+01
Temperature range (K), min.	296.92
Temperature range (K), max.	430.52

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C53897511&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume